

Generalized Geometrical Phase in the Case of Continuous Spectra

M. Maamache and Y. Saadi

*Laboratoire de Physique Quantique et Systèmes Dynamiques,
Faculté des Sciences, Université Ferhat Abbas de Sétif, Sétif 19000, Algeria*

Abstract

A quantal system in an eigenstate, of operators with a continuous nondegenerate eigenvalue spectrum, slowly transported round a circuit C by varying parameters in its Hamiltonian, will acquire a generalized geometrical phase factor. An explicit formula for a generalized geometrical phase is derived in terms of the eigenstates of the Hamiltonian. As an illustration the generalized geometrical phase is calculated for relativistic spinning particles in slowly-changing electromagnetic fields. It is shown that the the S-matrix and the usual scattering (with negligible reflexion) phase shift can be interpreted as a generalized geometrical phase.

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Historically, Berry's phase [1] has been introduced in the context of adiabatic evolution governed by an Hamiltonian $H(\vec{X}(t))$ whose parameters vary slowly in time and has been confined to discrete spectrum.

In quantum case, the adiabatic theorem concerns states $|\psi(t)\rangle$ satisfying the time-dependent Schrödinger equation and asserts that if a quantum system with a time-dependent non degenerate Hamiltonian $H(\vec{X}(t))$ is initially in the n th eigenstates of $H(\vec{X}(0))$, and if $H(\vec{X}(t))$ evolves slowly enough, then the state at time t will remain in the n th instantaneous eigenstates of $H(\vec{X}(t))$ up to a multiplicative phase factor $\phi_n(t)$. It has been shown [1], that there is an additional factor $e^{\gamma_n^B}$, a part from the familiar dynamical phase factor $e^{-\frac{i}{\hbar} \int E_n(t) dt}$ associated with the time evolution of the state being so transported with instantaneous eigenenergie $E_n(t)$, depending only the curve C which has been followed in the parameters space.

The question arises: is there a geometrical phase for a continuous spectrum? This case was raised for the first time by R. G. Newton [2] who looks at the S matrix as geometrical phase factor. Newton [2], introduced, what may be called the noninteraction picture to get the geometric phase factor in the continuous spectrum. In order to reinterpret the usual scattering phase shift as an adiabatic phase in the spirit of the original investigation of Berry, G. Ghosh [3] extends the adiabatic approximation to the continuous spectra like an anstaz confine themselves to one dimensional scattering with negligible reflection. Because the states are not normalizable and gauge invariance is lost, Ghosh [3] showed that the phase shift can be expanded in series of reparametrization invariant terms.

In this letter we give a generalization of the geometrical phase for the nondegenerate continuous spectrum. Three examples are worked out for illustration: -i) Dirac particle in a time-dependent electromagnetic field, -ii) The explicit relation between the geometrical phase and the S matrix with an example for application, -iii) the unidimensional reflectionless potential

Starting with the time-dependent Schrödinger equation governed by a Hamiltonian $H(\vec{X}(t))$ whose parameters vary slowly in time

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(\vec{X}(t)) |\psi(t)\rangle, \quad (1)$$

we define instantaneous eigenfunction in the continuous spectrum

$$H(\vec{X}(t)) |\varphi(k, t)\rangle = E(k, t) |\varphi(k, t)\rangle. \quad (2)$$

The adiabatic theorem demonstrated in Ref. [4], asserts that the evolved state of an initial Hamiltonian's eigenstate at time t_0

$$|\psi(t_0)\rangle = |\varphi(k, t_0)\rangle, \quad (3)$$

remains at any time t in the interval $[k, k + \delta k]$

$$|\psi(t)\rangle = \int_k^{k+\delta k} C(k'; t) |\varphi(k'; t)\rangle dk'. \quad (4)$$

Inserting (4) in the Schrödinger equation (1), lead to

$$\int_k^{k+\delta k} C(k'; t) E(k'; t) |\varphi(k'; t)\rangle dk' = \int_k^{k+\delta k} i\hbar \dot{C}(k'; t) |\varphi(k'; t)\rangle dk' + \int_k^{k+\delta k} i\hbar C(k'; t) |\dot{\varphi}(k'; t)\rangle dk' \quad (5)$$

where the dot stands for time-derivative. We multiply Eq. (5) by the bra of the eigendifferential [4]

$$\langle \delta\varphi(k; t) | = \int_k^{k+\delta k} \langle \varphi(k'; t) | dk', \quad (6)$$

this yields

$$\int_k^{k+\delta k} C(k'; t) E(k'; t) dk' = \int_k^{k+\delta k} i\hbar \dot{C}(k'; t) dk' + \int_k^{k+\delta k} C(k'; t) \langle \delta\varphi(k; t) | i\hbar \frac{\partial}{\partial t} |\varphi(k'; t)\rangle dk'. \quad (7)$$

Since k can sweep all the possible values and the intervals δk should be small ($\delta k \rightarrow 0$), the equality (7) between integrals implies the equality between integrands, hence

$$i\hbar \dot{C}(k'; t) = C(k'; t) \left[E(k'; t) - \langle \delta\varphi(k; t) | i\hbar \frac{\partial}{\partial t} |\varphi(k'; t)\rangle \right], \quad k' \in [k, k + \delta k]. \quad (8)$$

This equation is easily integrated and gives:

$$C(k'; t) = \delta(k' - k) \exp \left[- \int_{t_0}^t \left(\frac{i}{\hbar} E(k'; t') + \langle \delta\varphi(k; t') | i\hbar \frac{\partial}{\partial t'} |\varphi(k'; t')\rangle \right) dt' \right], \quad k' \in [k, k + \delta k], \quad (9)$$

hence

$$|\psi(k, t)\rangle = \exp \left\{ \frac{i}{\hbar} [-\gamma^D(k; t) + \gamma^G(k; t)] \right\} |\varphi(k; t)\rangle, \quad (10)$$

where $\gamma^D(k; t)$ is the familiar dynamical phase factor, and $\gamma^G(k; t)$ given by

$$\gamma^G(k; t) = \int_{t_0}^t \langle \delta\varphi(k; t') | i\hbar \frac{\partial}{\partial t'} |\varphi(k; t')\rangle dt', \quad (11)$$

is the generalization of the Berry's phase for the continuous spectrum. Note that all properties of the geometrical phase in discrete case are fulfilled by the generalized geometrical phase (11) for the continuous case.

As the interval $[k, k + \delta k]$ is located inside of the interval $[-\infty, +\infty]$, we can write the generalized geometrical phase in the following practical form

$$\gamma^G(k; t) = \int_{t_0}^t \int_{-\infty}^{+\infty} \langle \varphi(k'; t') | i\hbar \frac{\partial}{\partial t'} |\varphi(k; t')\rangle dt' dk', \quad (12)$$

which embodies the central result of this paper.

We now want to analyse the nature of the phase(12) through examples. Our first case is (i) the Dirac particle in a time-dependent electromagnetic field [5, 6], where the Dirac Hamiltonian in a 4-dimensional Hilbert space spanned by the two-dimensional basis state $|1\rangle$ and $|2\rangle$, can be written

$$H_D(t) = m(t) c^2 [|1\rangle \langle 1| - |2\rangle \langle 2|] + c \sigma^3 [p - f(t)] |1\rangle \langle 2| + c \sigma^3 [p - f^*(t)] |2\rangle \langle 1|, \quad (13)$$

p is the momentum operator, the mass $m(t)$ and the complex parameter $f(t)$ are periodic slowly functions of time, and σ^3 is the 2×2 standard Pauli matrix. In this way $|\psi(t)\rangle$ is a 4-dimensional spinor state. In fact, in the nonrelativistic limit [5], this Hamiltonian reduces to a Hamiltonian of charged particle interacting with an electromagnetic field in the so-called dipole approximation, i.e., the vector potential $eA(t) = \text{Re } f(t)$ and the scalar potential $eV(t) = \frac{\text{Im } f(t)}{2m(t)}$ are only functions of time but do not depend on coordinates.

At any time t , the instantaneous normalized, to δ -Dirac function, eigenstates of the Hamiltonian (13) are

$$|\varphi^\pm(z, k; t)\rangle = \left\{ \frac{c\sigma^3 g(k; t)}{\sqrt{[m(t)c^2 \mp \hbar\omega(k; t)]^2 + |g(k; t)|^2 c^2}} |1\rangle + \frac{m(t)c^2 \mp \hbar\omega(k; t)}{\sqrt{[m(t)c^2 \mp \hbar\omega(k; t)]^2 + |g(k; t)|^2 c^2}} |2\rangle \right\} \frac{e^{\frac{i}{\hbar}kz}}{\sqrt{2\pi\hbar}} \quad (14)$$

corresponding, respectively, to the eigenvalues $\pm\hbar\omega(k, t) = \pm c\sqrt{m^2(t)c^2 + |g(k; t)|^2}$ and $g(k; t) = f(t) - k$.

Substituting (14) in Eq. (12) leads to

$$\gamma^G(k; t) = \frac{i\hbar c^2}{2} \int_{t_0}^t \frac{g^*(k; t') \dot{g}(k; t') - \dot{g}^*(k; t') g(k; t')}{[m(t)c^2 \mp \hbar\omega(k; t)]^2 + |g(k; t)|^2 c^2} dt', \quad (15)$$

when we use the following representation of the adiabatic parameters $(\text{Re } f(t) - k)c = \hbar\omega \sin \theta \cos \varphi$, $\text{Im } f(t)c =$

Figure 1: Solid angle subtended by the circuit C .

$\hbar\omega \sin \theta \sin \varphi$ and $m(t)c^2 = \hbar\omega \cos \theta$; ω , θ and φ are now chosen as time-dependent adiabatic quantities, the generalized geometrical phase is nothing but the solid angle subtended by the circuit C when seen from $(k, 0, 0)$ in $(\text{Re } f(t), \text{Im } f(t), m(t)c)$ space (see Fig.1), i.e.

$$\gamma^G(k; C) = -\frac{\hbar}{2}\Omega. \quad (16)$$

Our next example is: (ii) the geometrical aspect of the S matrix: A very general way of looking at the S matrix as a geometric phase factor has been implicitly provided by Newton [2]. The expression for geometrical phase given in [2] looks strikingly similar to the equation of the wave operator in the interaction picture, which leads Newton to conclude that the S matrix appears in geometric phase as an expression of the adiabatic switching on and off of the interaction. Here we show explicitly that, in the case of an elastic scattering, the generalized geometrical phase (12) is nothing but the diagonal element of the S matrix.

The state vector $|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle$ of the given physical system is assumed to satisfy the Schrödinger equation (1), $U(t, t_0)$ being the unitary evolution operator associated to the Hamiltonian operator $H(t)$. In order to solve Eq. (1) under the adiabatic assumption, we assume that the Hamiltonian can be split into two parts

$$H(t) = H_0 + V(t), \quad (17)$$

so that H_0 represents the particles Hamiltonian in the absence of interaction between them. In other words, H_0 represents the free Hamiltonian operator. For the present we have primarily elastic scattering in mind, and we may think of $V(t)$ as the time-dependent potential of interaction. We assume that $V(t)$ varies slowly in time with

$$V(t) \neq 0 \quad t_0 < t < t_1. \quad (18)$$

In scattering problems, we are interested in calculating transition amplitudes between states $|\varphi^F(k)\rangle$ (where F stands for free evolution). The system initially in the state

$$|\psi(-\infty)\rangle = |\varphi^F(k_0)\rangle \quad (19)$$

evolves freely toward the interaction region as

$$|\psi(t)\rangle = \exp \left[-\frac{i}{\hbar} \int_{-\infty}^{t \leq t_0} E(k_0) dt' \right] |\varphi^F(k_0)\rangle, \quad (20a)$$

under the action of the free Hamiltonian H_0 whose eigenstates in the continuous spectrum are defined as

$$H_0 |\varphi^F(k)\rangle = E(k) |\varphi^F(k)\rangle. \quad (21)$$

Let us now expand the state vector $|\psi(t)\rangle$ on the basis of the instantaneous eigenstates $|\varphi(k, t)\rangle$ of $H(t)$ in the continuous spectrum

$$|\psi(t)\rangle = \int C^{ad}(k; t) |\varphi(k; t)\rangle dk, \quad (22)$$

(where ad stands for adiabatic evolution).

Expansion of $|\psi(t)\rangle$ on the basis of the instantaneous eigenstates $|\varphi^F(k)\rangle$ of H_0 leads to

$$|\psi(t)\rangle = \int C^F(k; t) |\varphi^F(k)\rangle dk \quad (23)$$

from which we may conclude by comparison with (22) that

$$C^F(k; t) = \int C^{ad}(k'; t) \langle \varphi^F(k) | \varphi(k'; t) \rangle dk', \quad (24)$$

with the initial condition (19), i.e. $C^F(k; -\infty) = \delta(k - k_0)$.

The coefficients $C^F(k; t)$ represent the matrix elements of the evolution operator $U(t, t_0)$ in the basis $\{|\varphi^F(k)\rangle\}$

$$C^F(k; t) = \exp \left[-\frac{i}{\hbar} \int_{-\infty}^t E(k_0) dt' \right] \langle \varphi^F(k) | U(t, t_0) | \varphi^F(k_0) \rangle. \quad (25)$$

In the interaction picture, the solution of the Schrödinger equation is transformed to

$$|\tilde{\psi}(t)\rangle = \exp \left[\frac{i}{\hbar} H_0 (t - t_0) \right] |\psi(t)\rangle. \quad (26)$$

The corresponding evolution operator $\tilde{U}(t, t_0)$ is related to the time-dependent unitary operator $U(t, t_0)$ by

$$\tilde{U}(t, t_0) = \exp \left[\frac{i}{\hbar} H_0 (t - t_0) \right] U(t, t_0). \quad (27)$$

It is easily verified that, by using (25) and (26), the matrix elements of this time-dependent operator between the eigenstates of the unperturbed Hamiltonian H_0 satisfy

$$\langle \varphi^F(k) | \tilde{U}(t, t_0) | \varphi^F(k_0) \rangle = C^F(k; t) \exp \left[\frac{i}{\hbar} \left(E(k)(t - t_0) + \int_{-\infty}^{t_0} E(k_0) dt' \right) \right]. \quad (28)$$

Let us now insert (9) in (24), this yields, taking into account that the collision is elastic and the initial condition here is given by (19),

$$C^F(k; t) = \langle \varphi^F(k) | \varphi(k_0; t) \rangle \exp \left[-\frac{i}{\hbar} E(k_0)(t - t_0) - \int_{t_0}^t \langle \delta\varphi(k_0; t') | \frac{\partial}{\partial t'} | \varphi(k_0; t') \rangle dt' \right]. \quad (29)$$

Comparison of (28) with (29) reveals that

$$\langle \varphi^F(k) | \tilde{U}(t, t_0) | \varphi^F(k_0) \rangle = \langle \varphi^F(k) | \varphi(k_0; t) \rangle \exp \left[\frac{i}{\hbar} \int_{-\infty}^{t_0} E(k_0) dt' - \int_{t_0}^t \langle \delta\varphi(k_0; t') | \frac{\partial}{\partial t'} | \varphi(k_0; t') \rangle dt' \right]. \quad (30)$$

As expected, the initial ($t \leq t_0$) and final ($t \geq t_1$) eigenstates of the free Hamiltonian H_0 are identical, i.e.

$$|\varphi^F(k_0, t \geq t_1)\rangle = |\varphi^F(k)\rangle. \quad (31)$$

By pushing the initial time into the distant past i.e. letting $t_0 \rightarrow -\infty$, similarly $t \rightarrow \infty$ signals that the scattering process is complete, we thus obtain the scattering matrix or S matrix

$$\langle \varphi^F(k) | S | \varphi^F(k_0) \rangle = \left\langle \varphi^F(k) \left| \lim_{t \rightarrow +\infty, t_0 \rightarrow -\infty} \tilde{U}(t, t_0) \right| \varphi^F(k_0) \right\rangle = \delta(k - k_0) \exp \left[\frac{i}{\hbar} \gamma^G(k_0; +\infty) \right] \quad (32)$$

On the basis of this comparison we may conclude that after the Hamiltonian completes an adiabatic circuit from H_0 via $H(t)$ back to H_0 , the state which initially was given by $|\varphi^F(k, t_0)\rangle$ has gone over into a new state that differs from it by a unitary transformation

$$S |\varphi^F(k)\rangle = S_k |\varphi^F(k)\rangle, \quad (33)$$

where S_k is the eigenvalue of the unitary S matrix and is related to the generalized geometrical phase (12) by

$$S_k = \exp \left[\frac{i}{\hbar} \gamma^G(k; +\infty) \right]. \quad (34)$$

This result expresses the geometric aspect of the S matrix and represents the transmission amplitude $t(k)$ [4].

Our final example is: (iii) the unidimensional potential

$$V(x; t) = -\frac{\hbar^2 k_1^2}{m [\cosh[k_1(x - x_0(t))]]^2} \quad (35)$$

which is reflectionless for all values of the incident energy, where m is the particle's mass, k_1 a constant and $x_0(t)$ is a slowly time-dependent function satisfying $x_0(t) \xrightarrow[t \rightarrow +\infty]{} +\infty$. The potential $V(x; t)$ (35) has a single

bound state of energy $E_{k=k_1} = -\frac{\hbar^2 k_1^2}{2m}$ and whose exact positive energy solutions given by

$$\varphi(x, k; x_0(t)) = [ik - k_1 \tanh[k_1(x - x_0(t))]] \frac{e^{ik.x}}{\sqrt{2\pi}(k_1 + ik)}, \quad (36)$$

are normalized in terms of the eigendifferentials [7].

Inserting (36) in (12) we get

$$\gamma^G(k; +\infty) = \frac{2\hbar k_1 k}{k^2 + k_1^2}, \quad (37)$$

which gives according to (34)

$$S_k = t(k) = \exp \left[2i \frac{k_1 k_0}{k_0^2 + k_1^2} \right] = e^{i \delta_0}. \quad (38)$$

This agrees with the results for the transmission amplitude obtained by Ghosh [3] and is a good approximation (see fig.2) for the well known exact transmission amplitude [3]

$$t(k) = \exp \left[2i \arctan \left(\frac{k_1}{k} \right) \right] = e^{i\delta}, \quad (39)$$

obtained in the time independent case.

Figure 2: illustrates a good agreement between the exact value δ (solid line) of the argument of the transmission amplitude and δ_0 (dashed line) the value of the generalized geometrical phase . The interval $[-\sqrt{2}, \sqrt{2}]$ corresponds to discrete spectrum region .

References

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- [5] M. Maamache and H.Lakehal, Europhys. Lett. **67**, 695 (2004)
- [6] This example has been treated by one of us [5] for the non adiabatic case using the Lewis-Riesenfeld theory and where $f(t)$ is a real function of time. In this Ref. [5] it was shown that, in the adiabatic limit, a Berry's phase appears; in fact this is not true because $f(t)$ is real which leads to a vanishing Berry's phase. The example treated here, where $f(t)$ is a complex parameter, gives a non vanishing geometrical phase which is the solid angle.
- [7] The functions (36) are normalized in terms of the eigendifferentials (6), indeed

$$\langle \varphi(k, x_0) | \varphi(k', x_0) \rangle = \delta(k - k') - \frac{k_1}{\pi(k_1 - ik)(k_1 + ik')} \lim_{L \rightarrow \infty} \cos[(k - k')L]$$

the last term takes any values between -1 and $+1$. Now, replacing $\langle \varphi(k, x_0) |$ by the corresponding eigen-differential we get

$$\langle \delta \varphi(k, x_0) | \varphi(k', x_0) \rangle = \int_k^{k+\delta k} \delta(k'' - k') dk'' + \frac{k_1 \tanh[k_1(x - x_0)]}{2i\pi(k_1 - ik)(k_1 + ik')x} e^{i(k-k')x} (e^{-i\delta kx} - 1) \Big|_{-\infty}^{\infty}$$

since the second term vanishes, then we can choose $\lim_{L \rightarrow \infty} \cos[(k - k')L] = 0$ without ambiguity [8].

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